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Simulation of the Concrete Containing Palm Oil Fuel Ash and Metakaolin in Terms of Mechanical Properties

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Abstract

This research investigates the compressive and split tensile strength of concrete containing Palm Oil Fuel Ash (POFA) and Metakaolin (MK) by using simulation method and validate with experimental data. This study aims to validate the Abaqus finite element analysis (FEA) results with experimental data, investigates the mechanical behaviour of concrete that contains MK as an additive and POFA as a partial cement substitute and identify the optimal mix design for enhanced strength by replacing cement with specific ratios of POFA and MK. The compressive strength, force-bearing capacity, and stress-strain behaviour of concrete mixes made with POFA and MK in different ratios were assessed. The trustworthiness of the model was confirmed by the results, which indicated that experimental data closely matched FEA predictions made with Abaqus. In contrast to the control mix, moderate replacement levels of concrete mix containing 5% POFA and 10% MK showed improved mechanical properties, however higher POFA concentration resulted in decreased strength and ductility. These results highlight POFA and MK's potential as sustainable concrete substitutes, given that the ratios are properly adjusted. By showing how simulation and experimental approaches can work in tandem to assess performance, this study promotes the development of green building materials.

1. Introduction

Concrete consumption is projected to rise from 10 billion tonnes annually to 18 billion tonnes by 2050 due to population growth [1]. While concrete is valued for its strength, durability, and versatility, enhancing its sustainability remains a priority. Incorporating supplementary cementitious materials (SCMs) like Palm Oil Fuel Ash (POFA) and Metakaolin (MK) offers a solution. POFA, a byproduct of palm oil waste, is rich in amorphous silica and exhibits pozzolanic activity, forming additional calcium silicate hydrate (C-S-H) gel that improves concrete's strength and longevity while reducing environmental impact [2]. MK, derived from calcining kaolin clay, enhances compressive strength and resilience against chemical attacks, extending concrete's lifespan. This research employs Abaqus finite element analysis (FEA) software to simulate the mechanical properties of concrete incorporating POFA and MK. By defining custom material models and simulating loading conditions, the study aims to evaluate the impact of these materials on concrete's strength, durability, and sustainability.

Concrete is a key material in modern infrastructure, but its production contributes significantly to CO2 emissions, releasing 0.7–1.1 tonnes of CO2 per tonne of cement, or about 5% of global emissions. Incorporating supplementary cementitious materials (SCMs) like Metakaolin (MK) and Palm Oil Fuel Ash (POFA) can enhance concrete's mechanical properties and sustainability by reducing ecological impacts and energy-intensive cement usage. POFA, abundant in Malaysia, offers an environmentally friendly cement alternative, aligning with Sustainable Development Goals (SDGs) 9, 11, and 12. Despite the promise of SCMs, challenges remain in fully understanding their mechanical properties and optimizing concrete performance. Finite Element Analysis (FEA) aids in simulating concrete's complex behavior under various conditions, addressing issues like flexural and shear failures. This research emphasizes the potential of MK and POFA to improve structural performance while promoting sustainable construction practices. Cubes or cylinders made on the job site are often evaluated seven and twenty-eight days later. The strength of Portland cement concrete at this age is typically two-thirds of the strength needed at 28 days; the 7-day tests serve as a benchmark for the rate of hardening. The findings of a twenty-eight-day strength test are typically used for concrete quality control and acceptance, as well as to ascertain whether the delivered concrete mixture satisfies the contract parameters for strength. The average of at least two concrete samples created from the same concrete and analysed at the same 28-day age is known as the test result [7].

Because a highly reactive POFA demonstrates greater cementitious strength than a less reactive POFA, POFA reactivity is crucial in determining the quantity of cement replacement material [6]. This research simulates concrete containing Palm Oil Fuel Ash (POFA) as a cement replacement (5%, 10%, and 15%) and Metakaolin (MK) as an additive (10%) using Abaqus software. A total of 12 concrete samples, including cubes and cylinders, will be analyzed under tensile and compressive loading scenarios to evaluate the mechanical properties. The study aims to create and validate a finite element model to simulate and optimize the concrete mix design. The simulation process involves part creation, property definition, boundary conditions, meshing, job submission, and result visualization, focusing on static analysis through the Finite Element Method (FEM).

It has been demonstrated that MK, a highly reactive pozzolanic substance rich in silicon and aluminium, reacts with carbonates to create stabilised ettringite and carboaluminate phases. The system's performance can be further enhanced and the detrimental effect of calcium carbonate ($CaCO3$) on strength can be lessened by the combined action of MK and limestone [3]. The active aluminium oxide and silicon dioxide contained in the MK can react with calcium hydroxide to produce C-S-H gel and hydrated calcium aluminate and hydrated calcium sulfoaluminate. This changes the material from disordered and flocculent to ordered and blocky, refines the pore space, enhances the pore structure of concrete, and increases densification [9].

Because of its silica concentration and pozzolanic activity, POFA is categorized as pozzolanic material. The primary component of POFA composition is silica which varies from 43.6% to 65.3% depending on the source, sample collection location, and burning temperature [1]. Concrete's flexural and crushing strengths can be increased by adding 15% MK to the mixture. In addition, it was found that MK concrete behaved better on measurements linked to concrete permeability [5].

While using Abaqus Software have to notice that the software is free in units. According to previous study, 'A comparative comparison of software packages for finite element analysis' from [8], it shows that Abaqus is free in units. This means that, any unit system such as SI, imperial, or custom can be used without requiring any configuration or switching. Ideal for a variety of technical specialities where various unit systems are frequently employed.

2. Methodology

The study employs finite element analysis to examine the mechanical properties of concrete containing Metakaolin (MK) and Palm Oil Fuel Ash (POFA). The methodology includes sample preparation, testing apparatus, data collection, and statistical analysis, ensuring accuracy and reliability. By detailing these processes, the research promotes transparency and enables replication, providing a foundation for further studies on sustainable and optimized concrete materials.

2.1 Concrete Properties

The study uses Finite Element Analysis (FEA) with a 3D nonlinear material model in the Abaqus explicit module to analyze concrete containing 5%, 10%, and 15% POFA as cement replacement and 10% MK as an additive. Both cube and cylinder samples were tested using the same structural model.

Table 1: Element Used for Concrete

No.	Part	Element	Definition
1	Concrete	C3D8R	An 8-node linear brick

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Cube concrete (150 mm x 150 mm x 150 mm) and cylinder concrete (150 mm x 300 mm) specimens were prepared. Each specimen was replicated to evaluate the effects of these material combinations. The density and elastic parameters for POFA-MK concrete were calculated using the material data gathered from the lab experiment and fed into the model. Tables 2 and 3 display the POFA-MK concrete cube and cylinder's Young's modulus (E), mass density (ρ), and Poisson ratio (v) from the experiment.

***Table 2*: Properties of POFA-MK cube concrete**

Type Concrete	Percentage of POFA	Percentage of MK	Young's Modulus, *E* (Pa)	Mass Density, P (kg/m^3)	Poisson's Ratio, *v*
MK-POFA Concrete 1	0%	0%	7767911497	2241.97	0.15
MK-POFA Concrete 2	5%	10%	6467860450	2232.10	0.15
MK-POFA Concrete 3	10%	10%	10143888270	2217.28	0.15
MK-POFA Concrete 4	15%	10%	13776252720	2000.00	0.16

***Table 3*: Properties of POFA-MK cylinder concrete**

Type Concrete	Percentage of POFA	Percentage of MK	Young's Modulus, *E* (Pa)	Mass Density, P (kg/m^3)	Poisson's Ratio, *v*
MK-POFA Concrete 1	0%	0%	7767911497	2282.59	0.11
MK-POFA Concrete 2	5%	10%	6467860450	2119.10	0.13
MK-POFA Concrete 3	10%	10%	10143888270	2144.25	0.13
MK-POFA Concrete 4	15%	10%	13776252720	2156.83	0.12

There are 4 different material properties, including regular concrete and POFA-MK concrete with variable concentrations of POFA and MK as added materials, were assessed, as indicated in Tables 2 and 3.

2.2 Modelling of Concrete

The cube and cylinder concrete were modeled using a 3D nonlinear material model with static analysis in the Abaqus explicit module. The same structural model was applied to analyze concrete properties with varying POFA replacement levels and 10% MK as an additive. Each specimen was independently simulated using Abaqus software for comprehensive evaluation.

The "Step" module in Abaqus manages the sequence of loading and boundary conditions in finite element analysis. Static and general step types were selected, with a 0.1 increment size and up to 100 increments. This process governs the simulation of concrete formation and loading conditions. Mesh discretization splits geometry into finite parts for simulation. Global seeds of size 15 were used, with C3D8R elements assigned to concrete. The Abaqus "Produce XY Data" module extracts simulation data, like stresses and displacements, for analysis. It exports results to Excel and creating plots and graphs for detailed evaluation.

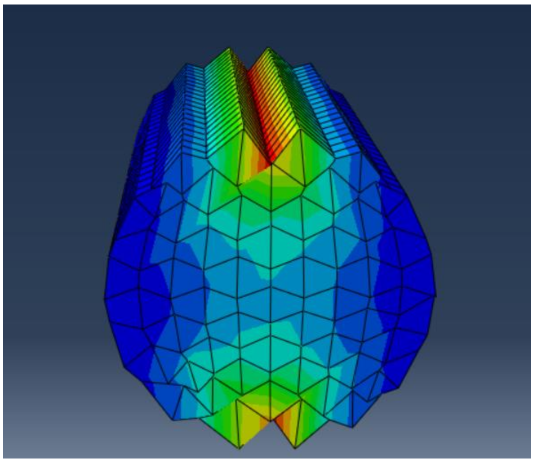

Fig. 1: Deformation Pattern of Concrete

3. Results and Discussion

Four models underwent static analysis to evaluate the compressive strength of cube and cylinder concrete and split tensile strength of cylinders. Performance data was analyzed, and graphs were created to compare concrete properties with varying MK-POFA percentages.

3.1 Abaqus Data

The outcomes of the Finite Element Analysis carried out with ABAQUS software were displayed based on Tables 4, 5, and 6.

Table 4: Compressive Strength of Cube Concrete

MK (%)	POFA (%)	Load (N)	Cross-Sectional Area (mm^2)	Compressive Strength (N/mm^2)
0	0	590003.63	22500	26.22
10	5	589511.63	22500	26.20
10	10	462281.72	22500	20.55
10	15	209528.23	22500	9.31

Table 5: Compressive Strength of Cylinder Concrete

MK (%)	POFA (%)	Load (N)	Cross-Sectional Area (mm^2)	Compressive Strength (N/mm^2)
0	0	439221.88	17671.46	24.85
10	5	325668.47	17671.46	18.43
10	10	499870.25	17671.46	28.29
10	15	693521.75	17671.46	39.25

Table 6: Split Tensile Strength of Cylinder Concrete

MK (%)	POFA (%)	Load (N)	Length (mm)	Diameter (mm)	Split Tensile Strength

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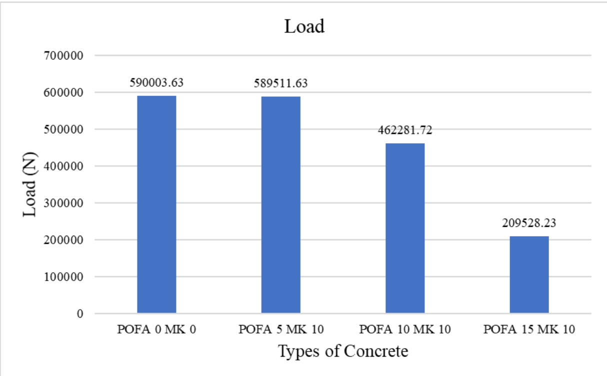
					(N/mm^2)
0	0	133596.13	300	150	1.89
10	5	165360.23	300	150	2.34
10	10	172895.69	300	150	2.45
10	15	117931.70	300	150	1.67

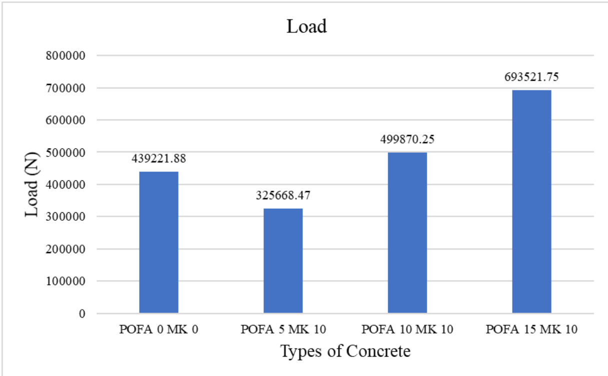
Tables above examines concrete mixtures containing Metakaolin (MK) and Palm Oil Fuel Ash (POFA) for their compressive strength and split tensile strength. A distinct percentage of POFA, ranging from 0% to 15% in 5% increments, is represented by each row.

3.2 Load

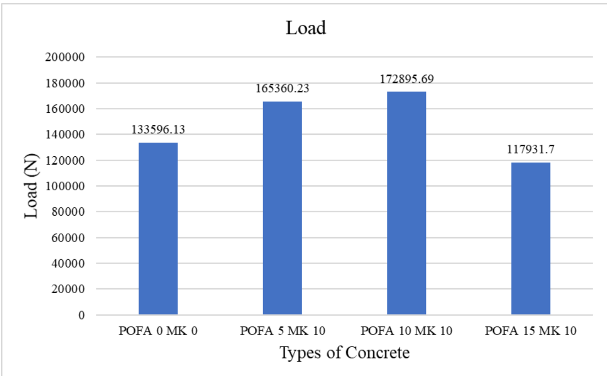
The load of cube concrete (compressive strength), load of cylinder concrete (compressive strength), and load of cylinder concrete (split tensile strength) are among the parameters that were examined.



(a)



(b)



(c)

Fig. 2: Loads for Cube Concrete (a) Cylinder Concrete (b) Cylinder Concrete in Split Tensile Strength (c)

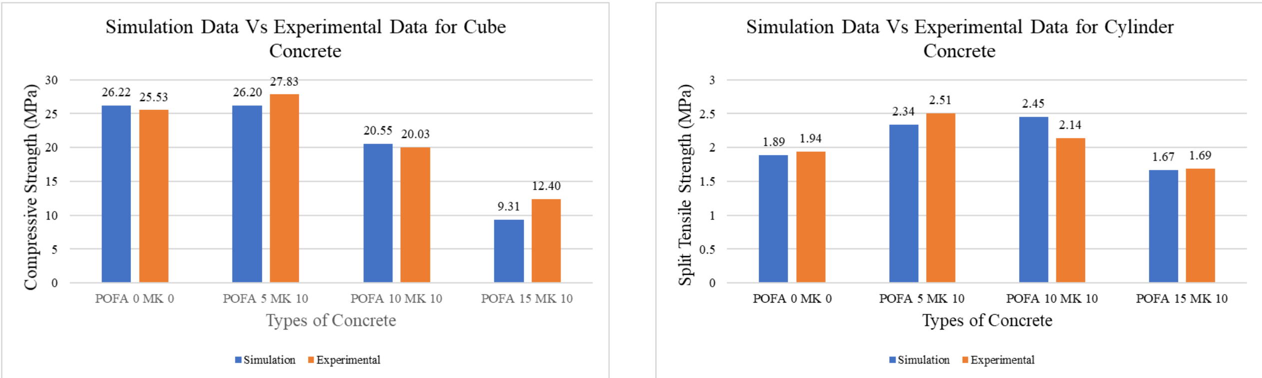
In Figure (a), the control mix (0% MK, 0% POFA) had the highest load capacity (590,003.63 N), while 5% POFA and 10% MK showed minimal reduction (589,511.63 N), indicating good synergy. Higher POFA levels (10%-15%) significantly reduced load capacity due to disrupted hydration. Optimal proportions, like 5% POFA and 10% MK, maintain strength, promote sustainability, and highlight POFA's potential as a partial cement substitute in construction.

In Figure (b), cylinder concrete results mirrored cube findings. The control mix (0% POFA, 0% MK) reached 439,221.88 N, while 5% POFA and 10% MK dropped to 325,668.47 N. Load peaked at 693,521.75 N with 15% POFA and 10% MK, surpassing the control by 58%, demonstrating the optimal synergy for enhancing compressive strength.

For Figure (c), the control mix (0% POFA, 0% MK) achieved a load capacity of 133,596.13 N. Concrete with 5% POFA and 10% MK increased capacity by 23.8% to 165,360.23 N, while 10% POFA and 10% MK peaked at 172,895.69 N (29.4% higher). Excessive POFA (15%) reduced capacity to 117,931.7 N. The optimal replacement is 10% POFA and 10% MK for improved mechanical performance.

3.3 Validation of Results between Simulation Data and Experimental Data

This section validates simulation results with experimental data by comparing the compressive strength of cube concrete and split tensile strength of cylinder concrete. Simulation accuracy is assessed using ABAQUS against laboratory results, ensuring reliability in predicting concrete behavior with POFA and MK. The validation also evaluates compliance with Grade 25 concrete standards (25 MPa after 28 days).



(a) (b)

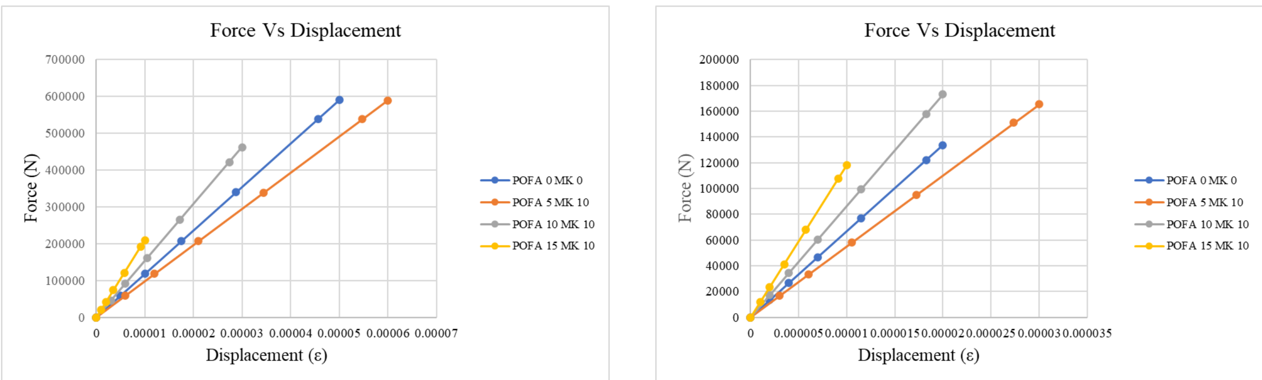
Fig. 3: Cube Compressive Strength (a) Cylinder Split Tensile Strength

The study validates simulation results against experimental data, in Fig.3 (a) with validation rates ranging from 2.6% to 24.92%. The control mix (0% POFA, 0% MK) showed a 2.7% validation rate, meeting the Grade 25 standard. Mixes with 5% POFA and 10% MK showed increased strength and a 2.6% validation rate, exceeding Grade 25 requirements. Higher POFA content (10% and 15%) reduced strength, with a validation rate of 24.92% for 15% POFA, highlighting the need for model refinement. Optimal mixes include up to 5% POFA and 10% MK.

For Fig.3 (b) the simulation model accurately predicted the split tensile strength of concrete with different POFA and MK proportions, showing validation rates of 2.58% (POFA 0%, MK 0%), 6.77% (POFA 5%, MK 10%), 14.49% (POFA 10%, MK 10%), and 1.18% (POFA 15%, MK 10%). POFA 15% MK 10% showed reduced tensile strength, indicating that higher POFA levels weaken matrix bonding and increase porosity. To improve accuracy, future studies could employ microstructural modelling methods such as the Lattice Discrete Particle Model (LDPM) or Discrete Element Method (DEM), which simulate particle interactions within the concrete matrix. The macroscopic tensile strength of concrete as determined by tensile splitting tests can be replicated using LDPM. It replicates the well splitting failure modes commonly seen in the trials and forecasts the impact of size on the tensile strength of concrete [4]. Overall, the model is reliable but requires refinement for mixes with higher POFA content to better account for pozzolanic effects and microstructural variations.

3.4 Force Vs Displacement

ABAQUS software has produced some force vs. displacement graphs from FEA. Three forces versus displacement plots, using cube and cylinder MK-POFA concrete, were displayed.



(a) (b)

Fig.4: Cube Concrete (a) Cylinder Concrete (b)

The study shows a proportional relationship between load and displacement for all mixes in Fig.4 (a). Maximum displacement and force decrease as POFA content rises, with POFA 0% MK 0% reaching 590,003.63 N and 0.00005, while POFA 15% MK 10% drops to 209,528.23 N and 0.00001. POFA 5% MK 10% exhibits slightly higher displacement (0.00006) than POFA 0% MK 0%, suggesting improved ductility. These results highlight that moderate POFA substitution (5%) maintains strength and enhances deformation behavior, but higher POFA levels (15%) significantly reduce mechanical performance, making them unsuitable for applications requiring high strength and ductility.

A proportional relationship between force and displacement, influenced by POFA and MK content in Fig.4 (b). The control sample achieves 133,596.13 N and 0.00002 displacement. POFA 5% MK 10% increases force by 23.74%, enhancing ductility, while POFA 10% MK 10% achieves the highest force at 172,895.69 N (29.36% improvement). Excessive POFA (15%) reduces force to 117,931.70 N, weakening bonds and hydration efficiency. Results underscore the importance of optimizing POFA and MK ratios to balance strength and ductility, with 5–10% POFA and 10% MK providing the best performance.

3.5 Stress Vs Strain

Out of all the combinations, the control sample has the highest stress, 26.22 MPa, showing higher compressive strength. The sample exhibits moderate ductility, deforming slightly prior to failure, as indicated by the strain value of 0.0075 at maximum stress. Conventional concrete exhibits this behaviour because its strength and stiffness are balanced.

With a strain of 0.009 at maximum stress, POFA 5% MK 10% cube concrete achieves a compressive strength that is similar to the control sample (26.20 MPa). The addition of MK and POFA, which increase the concrete's capacity to deform under stress without failing, is probably the cause of the increased strain, which indicates improved ductility. Applications needing both high strength and increased flexibility can use the blend. Fig. 5

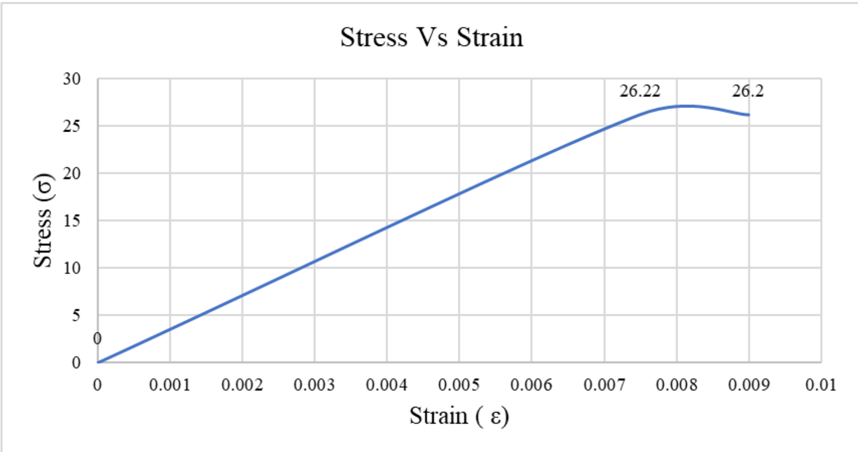


Fig. 5: Stress versus strain graph for cube concrete

3.6 Data Summary

The simulation and experimental results are summarized in Table 7 as shown.

Table 7: Summary of results for compressive and tensile strengths of concrete

Types of Concrete	Compressive Strength (MPa)		Split Tensile Strength (MPa)	
Cube	Simulation	Experimental	Simulation	Experimental
0% POFA 0% MK	26.22	25.53	-	-
5% POFA 10% MK	26.20	27.83	-	-
10% POFA 10% MK	20.55	20.03	-	-

15% POFA 10% MK	9.31	12.40	-	-
Cylinder	Simulation		Simulation	Experimental
0% POFA0% MK	24.85		1.89	1.94
5% POFA 10% MK	18.43		2.34	2.51
10% POFA 10% MK	28.29		2.45	2.14
15% POFA 10% MK	39.25		1.67	1.69

4. Conclusion

The study aimed to validate Abaqus Finite Element Analysis (FEA) results using experimental data, with compressive strength and stress-strain behavior experimental results closely matching the Abaqus FEA calculations, confirming the model's accuracy in predicting concrete's mechanical characteristics. The analysis of the mechanical properties under different loading situations, with varying POFA and MK ratios revealed that the combination of 5% POFA and 10% MK offered the best strength-ductility balance, while higher POFA concentrations (10%-15%) led to worse performance, underscoring the importance of selecting optimal replacement levels to meet structural requirements. Additionally, the study identified the ideal mix for enhanced strength and sustainability is concrete cylinder with 15% POFA and 10% MK as the validation rate is 1.18%. Reduced tensile strength resulted with an excessive POFA content (e.g., 15%), highlighting the necessity of cautious mix design.

5. Recommendations

Several suggestions are made based on the results and discussion of this study: Firstly, to enhance model accuracy and further validate Abaqus simulations, especially concerning microstructural effects, experimental research should be conducted. Secondly, the study should be expanded to include additional loading scenarios, such as dynamic and flexural loads, to comprehensively evaluate the performance of MK-POFA concrete. Lastly, practical guidelines should be provided for implementing the ideal mix design (10% MK and 10% POFA) in real construction projects, while promoting industry testing to verify the efficacy and scalability of the proposed mix design.

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Conflict of Interest

Authors declare that there is no conflict of interests regarding the publication of the paper.

Author Contribution

The authors confirm contribution to the paper as follows: ***study conception and design:*** *Low Yi Yun, Mohamad Hairi Bin Osman;* ***data collection:*** *Low Yi Yun, Aiman Iqbal Bin Yusaini;* ***analysis and interpretation of results:*** *Low Yi Yun;* ***draft manuscript preparation:*** *Low Yi Yun, Mohamad Hairi Bin Osman, Mohamad Luthfi Bin Ahmad Jeni. All authors reviewed the results and approved the final version of the manuscript.*

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